

Hexachlorophene  
70-30-4 | DTXSID6020690

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.90e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.67e-01

Confidence level: 3.12e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Hydroprene</div> <div>Measured: 3.39e-09</div> <div>Predicted: 8.80e-04</div>	<div>Image not found</div> <div>2-Propanone, 1,3-diphenyl-</div> <div>Measured: 7.53e-06</div> <div>Predicted: 3.07e-04</div>	<div>Image not found</div> <div>Methylcyclopentane</div> <div>Measured: 9.75e-11</div> <div>Predicted: 80.1</div>
<div>Image not found</div> <div>1-Nitroanthraquinone</div> <div>Measured: 5.00e-09</div> <div>Predicted: 9.88e-09</div>	<div>Image not found</div> <div>Thioglycolic acid</div> <div>Measured: 6.35e-09</div> <div>Predicted: 7.34e-02</div>	